

FINAL REPORT**Test Facility Study No. 511869****Determination of Physico-Chemical Properties of
MLA-3202**

- Melting and boiling temperature
- Density
- Vapour pressure
- Surface tension
- Flash-point
- Explosive properties
- Auto-ignition temperature
- Oxidizing properties
- Dissociation constants
- Appearance
- pH, acidity – alkalinity
- Viscosity
- Flammability in contact with water

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01 December 2016

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1. STATEMENT OF GLP COMPLIANCE

Charles River Den Bosch, 's-Hertogenbosch, The Netherlands

All phases of this study performed by the test facility were conducted in compliance with:

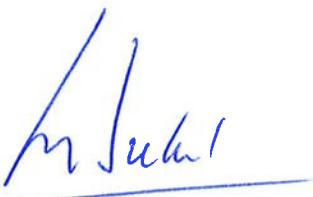
- OECD Principles of Good Laboratory Practice;
- EC Council Directive 2004 (2004/10/EC, February 11, 2004, Official Journal of February 20, 2004).

Except for the following:

- The test item characterization information supplied by the sponsor was produced under GLP.

The data generated and reported are considered to be valid.

Charles River Den Bosch



Signature:

Name: M.J.C. Brekelmans, MSc.

Title: Study Director

Date: December 01, 2016

2. TEST FACILITY QUALITY ASSURANCE STATEMENT

Charles River Den Bosch, 's-Hertogenbosch, The Netherlands

Study title: Determination of physico-chemical properties of MLA-3202.

This report was inspected by the Charles River Den Bosch Quality Assurance Unit (QAU) according to the Standard Operating Procedure(s).

The reported method and procedures were found to describe those used and the report reflects the raw data.

During the on-site process inspections, procedures applicable to this type of study were inspected.

The dates of Quality Assurance inspections are given below:

Project 511869

Type of Inspections	Phase/Process	Start Inspection date	End Inspection date	Reporting date to TFM and SD*
Study	Study Plan	23-May-2016	23-May-2016	23-May-2016
	Study Plan Amendment 01	08-Jun-2016	08-Jun-2016	08-Jun-2016
	Study Plan Amendment 02	11-Aug-2016	11-Aug-2016	11-Aug-2016
	Study Plan Amendment 03	14-Oct-2016	14-Oct-2016	14-Oct-2016
	Report	09-Nov-2016	09-Nov-2016	09-Nov-2016
Process	Analytical and physical chemistry	06-Jun-2016	21-Jun-2016	23-Jun-2016
	Test Item Handling			
	Exposure			
	Observations/Measurements			
Test Substance Receipt	Specimen Handling			
		22-Aug-2016	02-Sep-2016	09-Sep-2016
	Test Item Handling			
	Analytical and physical chemistry	05-Sep-2016	22-Sep-2016	30-Sep-2016
	Test Item Handling			
Exposure				
	Observations/Measurements			
Specimen Handling				

*TFM=Test Facility Management SD = Study Director

The review of the final report was completed on the date of signing this QA statement.

Charles River Den Bosch

Signature: A. Hout

Name: **Anita van Hout-Boudewijns, BSc**
Quality Assurance Auditor

Date: 30 nov 2016

3. SUMMARY

The results of the physico-chemical properties of the test item are given below.

Parameter	Guideline(s)	Result	Comment
Melting temperature	EC A.1 OECD 102 OPPTS 830.7200	-50 to +10°C (223 – 283 K)	
Boiling temperature	EC A.2 OECD 103 OPPTS 830.7220	no boiling temperature	reaction and/or decomposition of the test item at > 200°C (> 473K) was observed
Density	EC A.3 OECD 109 OPPTS 830.7300	D_4^{20} : 0.941	
Vapour pressure	EC A.4 OECD 104 OPPTS 830.7950	20°C 2.1×10^{-6} Pa = 1.6×10^{-8} mm Hg 25°C 4.6×10^{-6} Pa = 3.5×10^{-8} mm Hg	isothermal TGA effusion method
Surface tension	EC A.5 OECD 115	57.2 mN/m surface active	at 20°C by the harmonised ring method
Flash-point	EC A.9 UN p. 32.4.1 ASTM D 93 ASTM D7094 ISO 2719	no flash-point	closed cup method
Explosive properties	EC A.14 UN Test series 3 OPPTS 830.6316	not explosive	statement
Auto-ignition temperature	EC A.15 DIN 51794 IEC 79-4	360°C	at 1008.2 – 1015.5 hPa
Oxidizing properties	EC A.21 UN O.2	not oxidizing	statement
Dissociation constants	OECD 112 OPPTS 830.7370	No pKa in the pH range 1-13	Calculation method

Appearance			
Colour (Munsell code)	OPPTS 830.6302	Amber (8.75 YR 7/14)	
Physical state	OPPTS 830.6303	liquid	
Odour	OPPTS 830.6304	no odour noticed	
pH	CIPAC MT 75.3 OECD 122 OPPTS 830.7000	4.7 6.5	
Viscosity	OECD 114 OPPTS 830.7100 ISO 3104 ASTM D 445-09	1116 mm ² /s at 20°C 245 mm ² /s at 40°C	kinematic viscosity
Flammability (contact with water)	EC A.12 UN N.5	not highly flammable	statement

4. INTRODUCTION

4.1. Study schedule

Experimental starting date	22 June 2016
Experimental completion date	14 October 2016

4.2. Purpose of the study

The purpose of the study was to determine the following physico-chemical properties for MLA-3202:

- Melting and boiling temperature
- Density
- Vapour pressure
- Surface tension
- Flash-point
- Explosive properties
- Auto-ignition temperature
- Oxidizing properties
- Dissociation constants
- Appearance
- pH, acidity – alkalinity
- Viscosity
- Flammability in contact with water

4.3. Retention of records and materials

Records and material pertaining to the study, which include study plan and amendments, raw data and the final report will be retained in the archives of the test facility for a minimum of 5 years after the finalization of the report. After this period, the sponsor will be contacted to determine how the records and materials should be handled. The test facility will retain information concerning decisions made.

Perishable specimens (e.g. requiring refrigeration or freezing) will be discarded following evaluation in the study without further notice to the study sponsor.

A sample of the test item will be retained until expiry date or applicable retest date. After this period the sample(s) will be destroyed.

4.4. Responsible personnel

4.4.1. Test facility

Study Director	M.J.C. Brekelmans, MSc.
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4.4.2. Sponsor Representative

Study Monitor	Audrey Batoon, Ph.D.
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5. MATERIALS

5.1. Test item

5.1.1. Test item information

Test item	207258/A
Identification	MLA-3202
Appearance	Clear amber-red liquid
Batch	RC-1045
Purity/Composition	UVCB
Test item storage	At room temperature
Stable under storage conditions until	17 February 2019 (expiry date)

The certificate of analysis is shown in [Appendix 1](#).

5.1.2. Study specific test item information

Purity/composition correction factor	No correction factor required
Chemical name (IUPAC), synonym or trade name	Amides, tallow, N,N-bis(2-hydroxypropyl)
CAS Number	1454803-04-3
Test item handling	No specific handling conditions required

5.2. Electronic systems for data acquisition

System control, data acquisition and data processing were performed using the following program:

- Advantage Integrity Software version 3.0 (TA Instruments, New Castle, DE, USA)

Temperature, relative humidity and/or atmospheric pressure during sample storage and/or performance of the studies was monitored continuously using the following program:

- REES Centron Environmental Monitoring system version SQL 2.0 (REES Scientific, Trenton, NJ, USA)

5.3. List of deviations

5.3.1. List of study plan deviations

There were no deviations from the study plan.

5.3.2. List of standard operating procedures deviations

There were no deviations from standard operating procedures (SOPs).

6. MELTING AND BOILING TEMPERATURE

6.1. Guidelines

- European Community (EC), EC no. 440/2008, Part A: Methods for the Determination of Physico-Chemical Properties, Guideline A.1: "Melting/Freezing Temperature", Official Journal of the European Union no. L142, May 31, 2008.
- European Community (EC), EC no. 440/2008, Part A: Methods for the Determination of Physico-Chemical Properties, Guideline A.2: "Boiling Temperature", Official Journal of the European Union no. L142, May 31, 2008.
- Organization for Economic Co-operation and Development (OECD), OECD Guidelines for the Testing of Chemicals no. 102: "Melting Point / Melting Range", July 27, 1995.
- Organization for Economic Co-operation and Development (OECD), OECD Guidelines for the Testing of Chemicals no. 103: "Boiling Point", July 27, 1995.
- United States Environmental Protection Agency (EPA), Product Properties Test Guidelines no. OPPTS 830.7200: "Melting Point/Melting Range", March 1998.
- United States Environmental Protection Agency (EPA), Product Properties Test Guidelines no. OPPTS 830.7220: "Boiling Point/Boiling Range", August 1996.

6.2. Performance of the test

The melting and boiling temperature of the test item were determined using differential scanning calorimetry (DSC). This technique records the difference in heat flow of two crucibles, one filled with test item and the other left empty as reference, while these crucibles are subjected to a controlled temperature programme. A transition of the test item, such as melting or evaporation, is indicated by a deviation from the base line in the heat flow record. Because melting and evaporation are processes in which heat is consumed, the deviation from the base line is in the endothermic direction for these processes. The melting temperature or boiling temperature (if any) of the test item is evaluated from the DSC curve as the extrapolated onset temperature of the endothermic melting or evaporation peak.

As a safety precaution for the DSC cell a preliminary test was performed using a thermogravimetric analyzer (TGA).

6.2.1. Preliminary test

4.98 mg test item was heated at a rate of 20°C/minute from 25°C to 378°C. At this point 70% weight loss of the test item was observed. After the experiment, the sample was cooled to and equilibrated at 50°C and the consistency of the test item was determined.

6.2.2. Main study

An overview of the experimental conditions of the main study is given below.

Experiment	1	2
Sample amount (mg)	2.94	1.39
Initial temperature (°C)	25	25
Rate (°C/minute)	-5	-5
Temperature 2 (°C)	-90	-90
Rate (°C/minute)	20	20
End temperature (°C)	338	50

The experiments were performed under a flow of nitrogen and at atmospheric pressure.

6.3. Analytical method

Preliminary test

Instrument	Q50 thermogravimetric analyzer (TGA) (TA Instruments)
Sample container	aluminium; closed with a lid in which a small hole was drilled

Main study

Instrument	Q100 differential scanning calorimeter (TA Instruments, New Castle, DE, USA)
Sample container	aluminium; closed with a lid in which a small hole was drilled (used in Experiment 1 and 2)
Reference	empty sample container

6.4. Interpretation

The melting temperature is defined as the temperature at which the phase transition from solid to liquid state takes place at normal atmospheric pressure. This temperature ideally corresponds to the solidification or freezing temperature.

The standard boiling temperature is defined as the temperature at which the vapour pressure of a liquid is the same as the standard pressure (1013.25 hPa).

6.5. Results

6.5.1. Preliminary test

The TGA-curve of the test item is shown in [Figure 1](#). From 250°C upwards the weight of the sample decreased significantly. At 338°C the sample weight had decreased by 25%.

After the experiment, a brown residue remained in the sample container (original colour: amber-red). The change of the colour indicated reaction and/or decomposition of the test item.

6.5.2. Main study

The DSC-curve obtained with Experiment 1 is shown in [Figure 2](#). During cooling an exothermic peak was observed between -40°C and -10°C (results are archived in the raw data). The effect was obtained due to crystallization of the test item. During heating, an endothermic peak between -50°C and 25°C was observed. Due to an irregular baseline, caused by the composition of the test item (see Appendix 1), no defined melting temperature could be determined. Therefor a range was given for the melting temperature. Endothermic peaks were observed from 200°C. The effects were due to reaction and/or decomposition of the test item. After the experiment, a yellow residue remained in the sample container.

In order to obtain a sharper melting peak a lower heating rate of 5°C/minute was applied in the Experiment 2. [Figure 3](#) shows the DSC-curve obtained. The melting peak was observed between -50°C and +10°C but peal shape was still broad. After the experiment, a colourless residue remained in the sample container.

The melting range was determined from the width of the peak obtained with experiment 2 (between -50°C and 10°C).

6.6. Conclusion

The melting range of MLA-3202 was determined to be -50 to +10°C (223 – 283K) by using DSC.

Reaction and/or decomposition of MLA-3202 was observed during DSC experiment at temperatures of > 200°C (> 473K). Boiling of the test item was not observed below the temperature at which reaction and/or decomposition started. Based on this, the test item has no boiling temperature.

6.7. Figures

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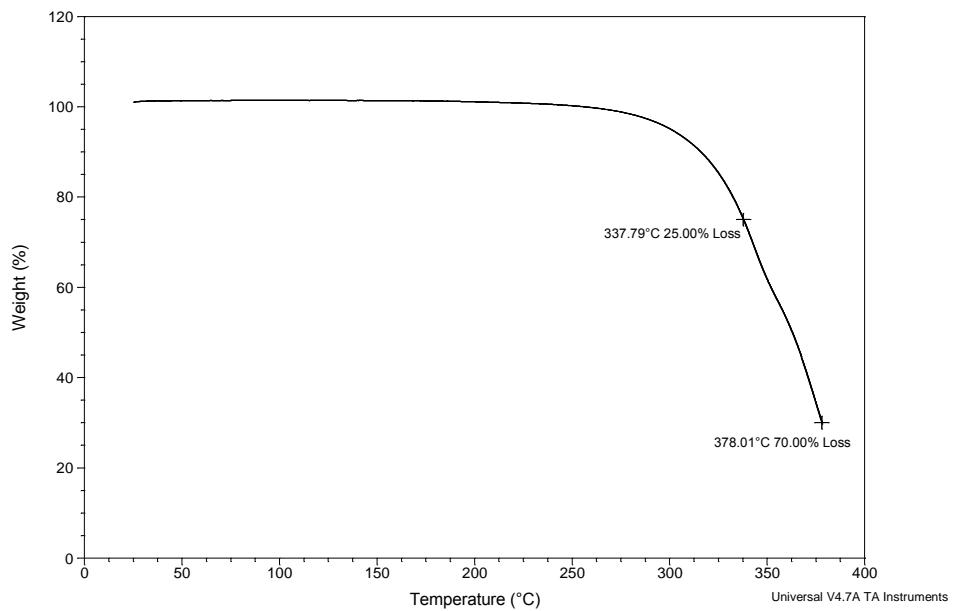


Figure 1
TGA curve of the test item

File: NOTOX2010 14672 88614

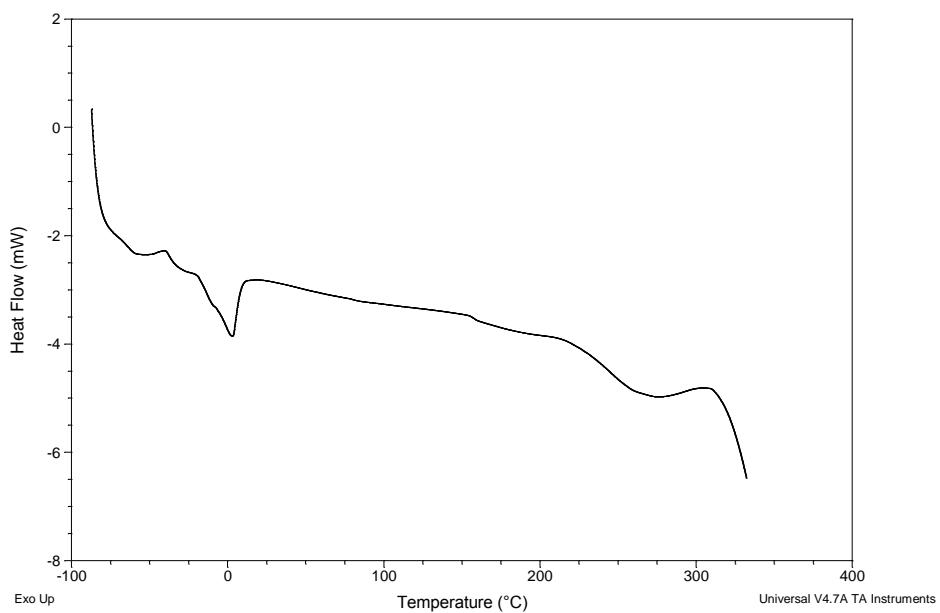


Figure 2
DSC curve of the test item obtained with Experiment 1

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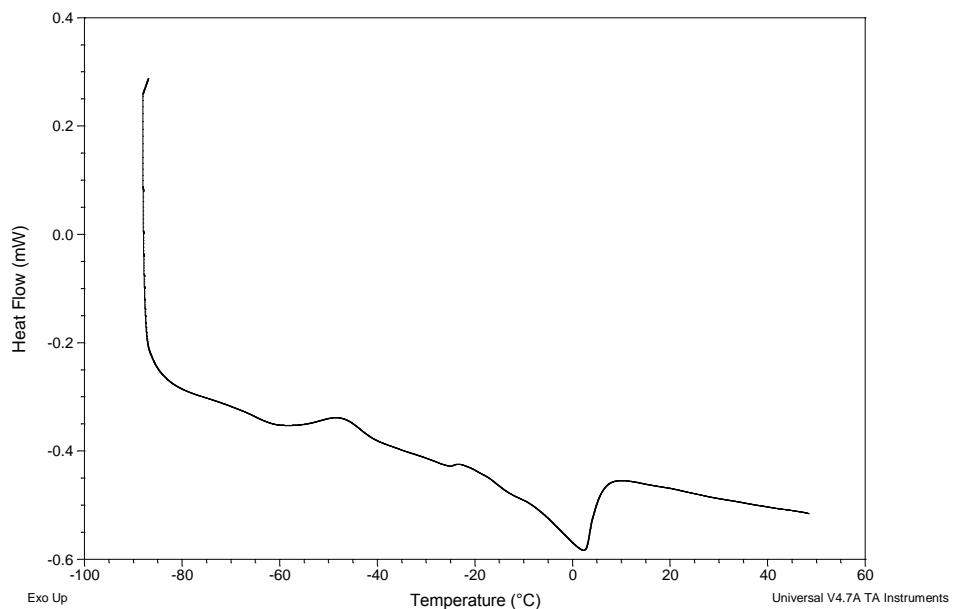


Figure 3
DSC curve of the test item obtained with the first heating of Experiment 2

7. DENSITY

7.1. Guidelines

- European Community (EC), EC no. 440/2008, Part A: Methods for the Determination of Physico-Chemical Properties, Guideline A.3: "Relative Density", Official Journal of the European Union no. L142, May 31, 2008.
- Organization for Economic Co-operation and Development (OECD), OECD Guideline for the Testing of Chemicals no. 109: "Density of Liquids and Solids", October 2, 2012.
- United States Environmental Protection Agency (EPA), Product Properties Test Guidelines no. OPPTS 830.7300: "Density/Relative Density/Bulk Density", June 2002.

7.2. Reagents

Water Tap water purified by a Milli-Q water purification system (Millipore, Bedford, MA, USA).

7.3. Performance of the study

The density (ρ) and relative density (D_4^{20}) of the test item were determined using a pycnometer with a volume of 10 mL. The density of the test item is calculated from the difference in weight between the full and empty pycnometer and its volume.

The volume of the pycnometer was determined first. The pycnometer was weighed empty. Then it was filled with water, dried on the outside and weighed again. The temperature of the water was measured. The procedure was performed in duplicate. The mean volume of the pycnometer was calculated.

The pycnometer was filled with test item, dried on the outside and weighed. The temperature of the test item was measured. The test was performed in duplicate. The mean density and relative density of the test item were determined.

Measurements were performed at $20.0 \pm 0.5^\circ\text{C}$. Weightings were performed on an analytical balance with an accuracy of 0.1 mg.

7.4. Interpretation

The density (ρ) of a substance is the quotient of its mass and its volume and is expressed in SI units of kg/m^3 .

The relative density (D_4^{20}) is the ratio between the mass of a volume of a substance to be examined, determined at 20°C , and the mass of the same volume of water, determined at 4°C ($\rho_{\text{H}_2\text{O}}^4 = 1000 \text{ kg}/\text{m}^3$). The relative density has no dimension.

$$\text{Volume of the pycnometer (V)} \quad V = \frac{B - A}{\rho_{\text{H}_2\text{O}}^{20}} \quad [\text{cm}^3]$$

where:

A = weight of the empty pycnometer [g]

B = weight of the pycnometer with water [g]

$\rho_{\text{H}_2\text{O}}^{20}$ = density of water at 20°C i.e. $0.9982 \text{ g}/\text{cm}^3$

(CRC Handbook of Chemistry and Physics, 1981)

$$\rho = \frac{C - A_{\text{mean}}}{V_{\text{mean}}} \text{ [g/cm}^3\text{]}$$

where:

C = weight of the pycnometer with test item [g]

7.5. Results

[Table 1](#) shows the determined volume of the pycnometer. The results of the tests on the determination of the density of the test item are given in [Table 2](#).

The individual measurements were obtained with a deviation of $\leq 0.01 \text{ g/cm}^3$. According to the guideline, the density of the test item is given as the mean value.

Table 1
Determination of the volume of the pycnometer

	Test 1	Test 2	Mean
Mass empty pycnometer (A)	30.4760 g	30.4760 g	30.4760 g
Mass pycnometer with water (B)	40.1104 g	40.1110 g	
Volume of the pycnometer	9.6518 cm ³	9.6524 cm ³	9.6521 cm ³

Table 2
Density of the test item

	Test 1	Test 2	Mean
Mass pycnometer with test item (C)	39.5524 g	39.5584 g	
Density	0.9404 g/cm ³	0.9410 g/cm ³	0.941 g/cm ³

7.6. Conclusion

A pycnometer was used for the determination of the density and relative density of MLA-3202.

The density of the test item at 20°C was 0.941 g/cm³ ($0.941 \times 10^3 \text{ kg/m}^3$).

The relative density was 0.941.

8. VAPOUR PRESSURE

8.1. Guidelines

- European Community (EC), EC no. 761/2009, Part A: Methods for the Determination of Physico-Chemical Properties, Guideline A.4: "Vapour Pressure", Official Journal of the European Union no. L220, August 24, 2009.
- Organization for Economic Co-operation and Development (OECD), OECD Guidelines for the Testing of Chemicals no.104: "Vapour Pressure", March 23, 2006.
- United States Environmental Protection Agency (EPA), Product Properties Test Guidelines no. OPPTS 830.7950: "Vapor pressure", August 1996.

8.2. Performance of the test

The vapour pressure of the test item (P_T) was determined by the isothermal thermogravimetric effusion method. The method is validated in the range $10^{-8} - 10^3$ Pa using a set of five reference substances with known vapour pressures (see paragraph 0). The validity of the method was verified maximum one month before this study using hexachlorobenzene as reference control substance. Since the logarithm of the evaporation rate at 20°C ($\log v_{T, 20}$) deviated < 10% from the average value obtained during the validation test, it was possible to apply the constants obtained with the validation test for the determination of the vapour pressure of the test item.

An amount of 7.63 or 10.5 mg of the test item was applied to the surface of a roughened glass plate as a homogeneous layer.

The following temperature program was applied. The weight loss of the test item was measured continuously as a function of time.

Start temperature	30°C
Isothermal intervals	10 minutes
Increment steps	10°C
End temperature	200°C

The weight loss of the test item was measured continuously as a function of time at defined isothermal temperatures. The evaporation rate of the test item (v_T) was calculated from the weight loss of the compound. The P_T values at the defined isothermal temperatures were determined using the vapour pressure equation with the constants c and d specific for the experimental arrangement. Linear regression analysis of the $\log P_T$ values and $1/T$ was performed using a least squares method. The P_T values of the test item at 20°C and 25°C were determined using the vapour pressure regression curve.

8.3. Analytical method

Instrument Q50 thermogravimetric analyzer (TGA)
(TA Instruments, New Castle, DE, USA)

Surface of the glass plate 0.50 cm²

The experiments were performed under a flow of nitrogen and at atmospheric pressure.

8.4. Reference substances

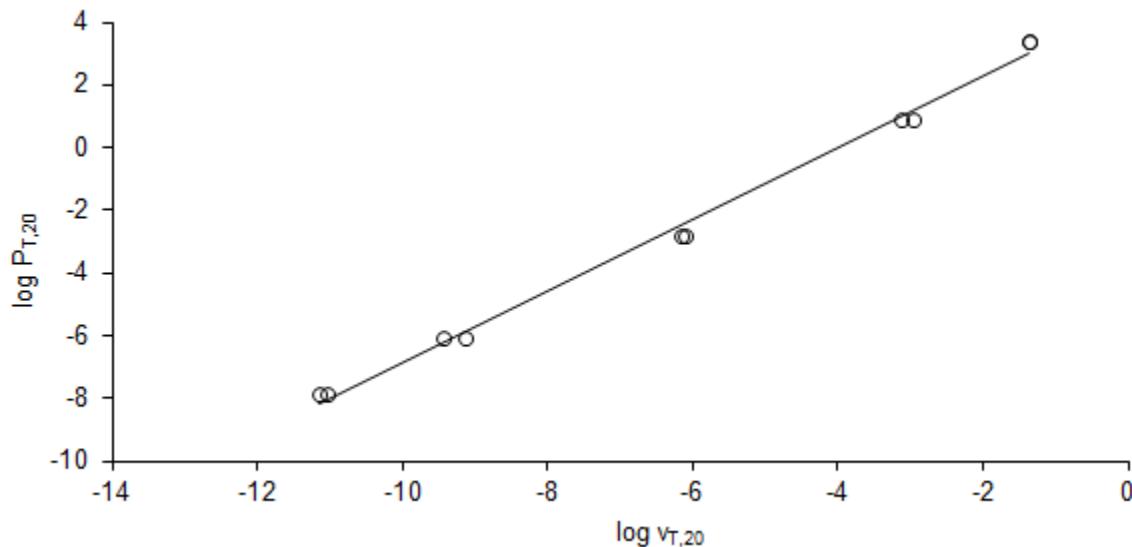
Validation of the method is performed at least once every year (project 512159).

Each reference substance was measured in duplicate by TGA using a temperature program that was specific for the substance. Plots of $\log vT$ obtained at elevated temperatures and $1/T$ were inter- or extrapolated to determine the $\log vT$ values at 20°C ($\log vT_{,20}$). The $\log vT_{,20}$ values were plotted against the logarithm of the vapour pressure at 20°C in Pascal units ($\log PT_{,20}$). Linear regression analysis using the least squares method yielded an equation of $\log PT_{,20} = 1.14 \times \log vT_{,20} + 4.55$. The coefficient of correlation (r) was > 0.99 . The constants c and d specific for the experimental arrangement were 1.14 and 4.55, respectively.

Reference substance	Reference P_T values 20°C		Corresponding P_T values 25°C		Literature
	[Pa]	[mm Hg]	[Pa]	[mm Hg]	
Benzo(ghi)perylene	1.33×10^{-8}	1.00×10^{-10}	$1.90 \times 10^{-8}^{\#}$	$1.42 \times 10^{-10}^{\#}$	1
Chrysene	8.40×10^{-7}	6.30×10^{-9}	$2.03 \times 10^{-6}^{\#}$	$1.53 \times 10^{-8}^{\#}$	2
Hexachlorobenzene	1.47×10^{-3}	1.10×10^{-5}	$6.91 \times 10^{-3}^{\#}$	$5.19 \times 10^{-5}^{\#}$	1
Naphthalene	7.56×10^0	5.67×10^{-2}	1.15×10^1	8.61×10^{-2}	3
Water	2.34×10^3	1.75×10^1	3.17×10^3	2.38×10^1	3

Determined by the vapour pressure regression curve of the validation study. No literature value was available.

1. Verschueren, K., Handbook of environmental data on organic chemicals, 4th edition, Wiley Chemistry
2. Borges, H.T., Formal toxicity summary for Chrysene, The Risk Assessment Information System (RAIS), 1994
3. Lide, D.R., CRC Handbook of Chemistry and Physics, 79th edition, CRC Press LLC., Boca Raton, FL, USA, 1998



8.5. Interpretation

8.5.1. Specifications

The vapour pressure is a function of the temperature and is specified in Pascal (Pa) or in mm Hg.

8.5.2. Formulas

Evaporation rate (v_T)	$v_T = \frac{\Delta m}{F \times t}$ [g/cm ² /h]
	where: Δm = weight loss of the test item [g] F = surface of the sample plate [cm ²] t = elapsed time for the weight loss [h]
Vapour pressure equation	$\log P_T = c \log v_T + d$ where: c = constant specific for the experimental arrangement d = constant specific for the experimental arrangement
Vapour pressure regression curve	$\log P_T = a /T + b$ where: T = temperature [K] a = slope [K] b = intercept

8.6. Results

A representative weight loss curve of the test item is shown in [Figure 4](#). The results of the isothermal TGA analysis for the test item and the vapour pressure at 20°C and 25°C are given in [Table 3](#) and [Table 4](#).

The plot of the log P_T of the test item as function of the reciprocal temperatures is shown in [Figure 5](#). The equation of the curve was: $\log P_T = -6012 \times 1/T + 14.83$ ($r = 0.990$, $n = 8$).

Table 3
Results of the isothermal TGA analysis

Temperature [°C]	Weight loss [µg/min]	v _T [g/cm ² /h]	log v _T	log P _T	P _T [Pa]
160	5.653	6.75×10^{-4}	-3.17	0.93	8.6
	6.733	8.04×10^{-4}	-3.09	1.02	10
170	9.241	1.10×10^{-3}	-2.96	1.18	15
	11.20	1.34×10^{-3}	-2.87	1.27	19
180	18.08	2.16×10^{-3}	-2.67	1.51	32
	20.84	2.49×10^{-3}	-2.60	1.58	38
190	36.35	4.34×10^{-3}	-2.36	1.86	72
	38.49	4.59×10^{-3}	-2.34	1.88	77

Table 4
Vapour pressure of the test item

Temperature [°C]	log P _T	P _T [Pa]	P _T [mm Hg]
20	-5.68	2.1×10^{-6}	1.6×10^{-8}
25	-5.34	4.6×10^{-6}	3.5×10^{-8}

8.7. Conclusion

The isothermal TGA effusion method was applied for the determination of the vapour pressure of MLA-3202.

The vapour pressure of the test item at 20°C (293K) and 25°C (298K) was:

	20°C		25°C	
	[Pa]	[mm Hg]	[Pa]	[mm Hg]
Test item	2.1×10^{-6}	1.6×10^{-8}	4.6×10^{-6}	3.5×10^{-8}

8.8. Figures

File: NOTOX2010 14676 13036

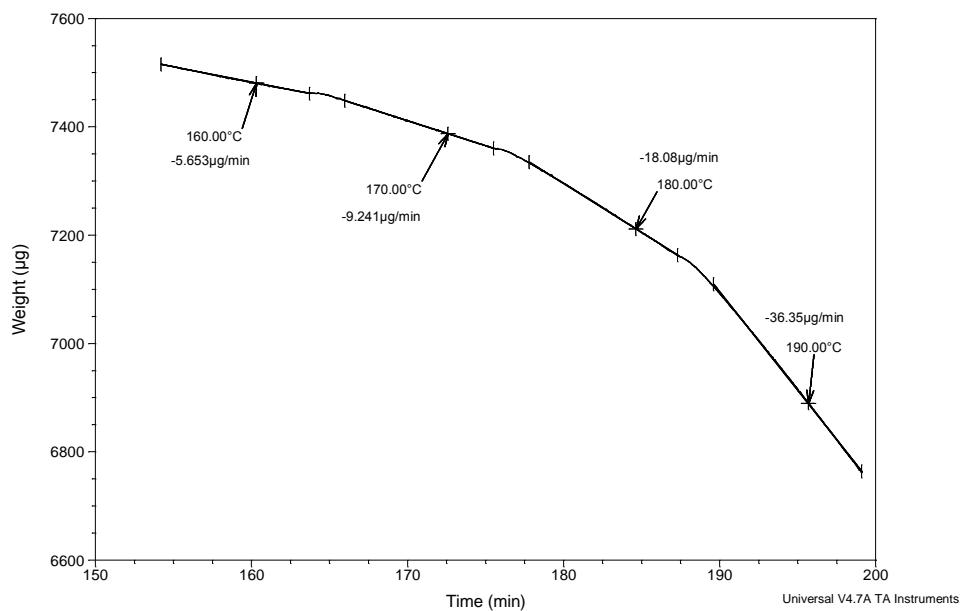


Figure 4
Weight loss curve of the test item.

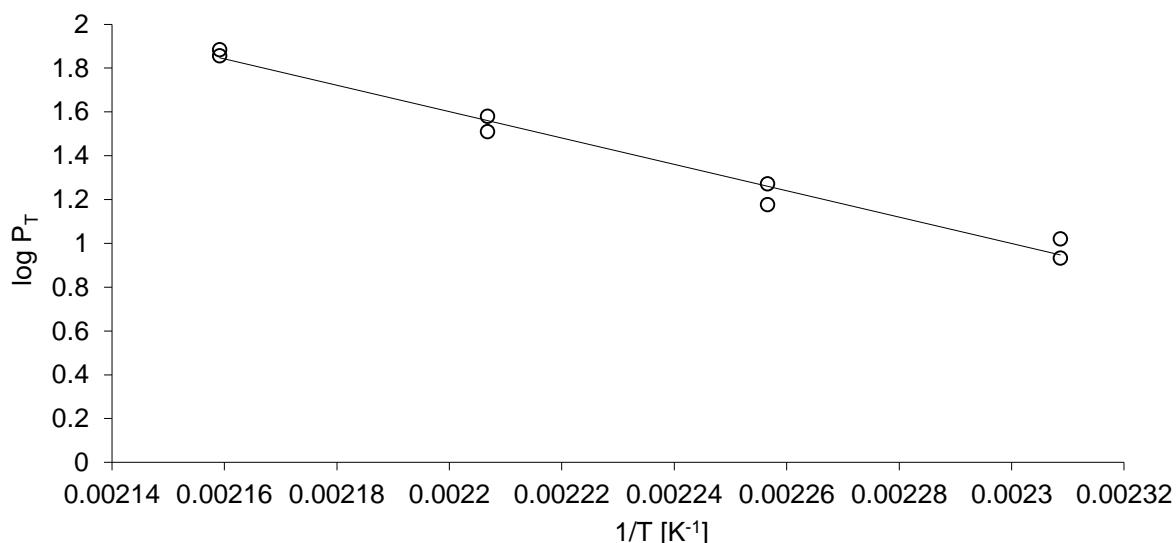


Figure 5
Plot of log Pt of the test item *versus* 1/T.

9. SURFACE TENSION

9.1. Guidelines

- European Community (EC), EC no. 440/2008, Part A: Methods for the Determination of Physico-Chemical Properties, Guideline A.5: "Surface Tension", Official Journal of the European Union no. L142, May 31, 2008.
- Organization for Economic Co-operation and Development (OECD), OECD Guidelines for the Testing of Chemicals no. 115: "Surface Tension of Aqueous Solutions", July 27, 1995.

9.2. Reagents

Double distilled water	Waldeck, Münster-Roxel, Germany
Methanol	Biosolve, Valkenswaard, The Netherlands
Chromosulfuric acid	for cleaning glass vessels, Merck, Darmstadt, Germany
<i>ortho</i> -Phosphoric acid, 85%	Merck

All reagents were of analytical grade, unless specified otherwise.

9.3. Performance of the study

The surface tension of the test item was determined using the OECD harmonized ring method. The system consists of the following elements: model K6 tensiometer (Krüss, Hamburg, Germany), platinum-iridium ring with a wire radius of 0.185 mm and a ring radius of 9.545 mm and a cylindrical glass vessel with an inside diameter of 45 mm.

All glassware was washed with hot chromosulfuric acid and subsequently with syrupy phosphoric acid, thoroughly rinsed in tap water and finally washed with double distilled water. The platinum-iridium ring was rinsed thoroughly in water, briefly immersed in chromosulfuric acid, washed with double distilled water and finally heated briefly above a methanol flame.

An aliquot of 201.4 mg of the test item was stirred with 200 mL double distilled water at $20.1 \pm 0.3^\circ\text{C}$ for 18 hours. After the stirring period, a sample of the suspension was centrifuged at 3500 g and 20°C for 5 minutes. In order to remove test item particles floating on the surface of the test sample, the solution was additionally filtered through a 0.45 μm Spartan 30/0.45 RC filter (Whatman, Dassel, Germany). Thereafter, 90 mL of the aqueous phase was mixed with 10 mL double distilled water to obtain the test solution at 90% of the test item saturation solubility in water.

The test solution at 90% of the test item saturation solubility in water was filtered through a 0.45 μm Spartan 30/0.45 RC filter (Whatman, Dassel, Germany). The cylindrical glass vessel was filled with water or test solution and placed in a vessel holder on a mobile sample table. The time between preparation of the test solution and transferring it to the vessel was 2 minutes. The mobile sample table was raised until the ring was immersed below the surface of the solution. The table was subsequently lowered until the ring was in contact with the liquid surface. The surface tension of the test item was determined using the tensiometer. Five measurements were performed until a constant value on the surface tension was reached ($< 0.5 \text{ mN/m}$). The time passed since the solution was transferred to the measurement vessel was measured for each measurement.

The test was performed at $20.0 \pm 0.5^\circ\text{C}$.

9.4. Calibration of the tensiometer

On the day of measurement the OECD harmonized ring method was calibrated using double distilled water. The results on the calibration experiments are given below. The test was performed at $20.0 \pm 0.5^{\circ}\text{C}$. The calibration factor (Φ_b) was calculated to be 0.99.

Measurement	Time passed after transfer calibration solution to test vessel [minutes]	Surface tension [mN/m]	
		individual	mean
1	16	73.7	73.6
2	17	73.6	
3	18	73.6	
4	19	73.5	
5	20	73.5	

9.5. Interpretation

A test item with a surface tension < 60 mN/m will be regarded as being a surface active material.

The mean surface tension of the test solution was multiplied by the calibration factor followed by correction according to Harkins-Jordan. Interpolation was used for readings ranging between the table values.

$$\text{Calibration factor } (\Phi_b) \quad \Phi_b = \frac{\sigma_o}{\sigma_m}$$

where:

σ_o = surface tension of water at the test temperature cited in the literature i.e. 72.74 mN/m at 20.0°C (Vargaftik, *et. al.*, J. Phys. Chem. Ref. Data 12, 817, 1983)

σ_m = mean surface tension of double distilled water obtained on the day of measurement

Correction of the measured surface tension according to Harkins-Jordan

Experimental value [mN/m]	Corrected value [mN/m]	Experimental value [mN/m]	Corrected value [mN/m]
20	18.1	50	48.6
22	20.1	52	50.7
24	22.1	54	52.8
26	24.1	56	54.9
28	26.1	58	57.0
30	28.1	60	59.1
32	30.1	62	61.3
34	32.1	64	63.4
36	34.1	66	65.5
38	36.1	68	67.7
40	38.2	70	69.9
42	40.3	72	72.0
44	42.3	74	74
46	44.4	76	76
48	46.5	78	78

W.D. Harkins, H.F. Jordan, J. Amer. Chem. Soc., vol. 52, 1751, 1930.

9.6. Results

The results of the test on the determination of the surface tension of the test solution are given in [Table 5](#).

Table 5
Surface tension of the test item

Measurement	Time passed after transfer test solution to test vessel [minutes]	Surface tension [mN/m]		
		individual	mean	mean multiplied by Φ_b and Harkins- Jordan corrected value
1	18	58.6	58.8	57.2
2	19	58.9		
3	20	58.9		
4	21	58.8		
5	22	59.0		

9.7. Conclusion

The OECD harmonized ring method was applied for the determination of the surface tension of Amides, tallow, N,N-bis(2-hydroxypropyl).

The surface tension of a test solution at 90% of the test item saturation solubility in water and at 20°C was 57.2 mN/m. According to this, the test item is considered to be surface active.

10. FLASH-POINT

10.1. Guidelines

- European Community (EC), EC no. 440/2008, Part A: Methods for the Determination of Physico-Chemical Properties, Guideline A.9: "Flash-point", Official Journal of the European Union no. L142, May 31, 2008.
- United Nations (UN), UN no. ST/SG/AC.10/11/Rev.6: Recommendations on the Transport of Dangerous Goods, Part III: Classification Procedures, Test Methods and Criteria Relating to Class 2, Class 3, Class 4, Division 5.1, Class 8 and Class 9, Paragraph 32.4.1: "Non-Viscous Flammable Liquids", 2015.
- ASTM International, ASTM D93: "Standard Test Methods for Flash Point by Pensky-Martens Closed Cup Tester", December 10, 2002.
- ASTM International, ASTM D7094: "Standard Test Method for Flash Point by Modified Continuously Closed Cup (MCCCFP) Tester", 2012.
- The International Organization for Standardization (ISO), ISO Guide 2719: "Determination of Flash Point – Pensky-Martens closed cup method", 2002.

10.2. Performance of the test

The flash-point of the test item was determined using an Eraflash flash-point tester (Eralytics, Vienna, Austria). The Eraflash tester employs a small volume of test item which reduces the risk of fires or other uncontrolled reactions of substances with an unknown flash point. The test cup was filled with approximately 2 ml test item and placed in the holder of the flash-point tester. The test cup was put in the measurement chamber and the door was closed. The sample was stirred during heating. The ignition of the sample vapour was performed by an electric arc and ignition was automatically detected by the flash point tester. The flash-point is automatically corrected for atmospheric pressure by the flash point tester.

10.2.1. Preliminary test

The test cup was heated at a rate of $5 \pm 0.5^{\circ}\text{C}/\text{minute}$. Starting at 25°C , an attempt was made to ignite the vapour of the test item for every 2°C temperature rise.

A pressure error occurred at 261°C . The preliminary test was repeated and the same situation occurred at 269°C indicating that the test item does not have a flash point.

10.3. Interpretation

The flash-point of the test substance is the lowest temperature at which the test substance evolves vapours in such amount that a flammable vapour/air mixture is produced in the test vessel.

10.4. Results**10.4.1. Preliminary test**

No flammable vapour/air mixture was produced at temperatures below the temperature when a pressure error was observed. During the measurement, the hot flame of the ignited vapour did not cause an instantaneous pressure increase of at least 20 kPa inside the closed measuring chamber. From this, it was concluded that the test item has no flash point.

10.5. Conclusion

The closed cup method was applied for the determination of the flash-point of MLA-3202.

No flash-point was observed.

11. EXPLOSIVE PROPERTIES

11.1. Guidelines

- European Community (EC), EC no. 440/2008, Part A: Methods for the Determination of Physico-Chemical Properties, Guideline A.14: "Explosive Properties", Official Journal of the European Union no. L142, May 31, 2008.
- United Nations (UN), UN no. ST/SG/AC.10/11/Rev.6: Recommendations on the Transport of Dangerous Goods, Part I: Classification Procedures, Test Methods and Criteria Relating to Explosives of Class 1, Section 13: "Test Series 3", 2015.
- United Nations (UN), UN no. ST/SG/AC.10/11/Rev.6: Recommendations on the Transport of Dangerous Goods, Appendix 6: "Screening Procedures", 2015.
- United States Environmental Protection Agency (EPA), Product Properties Test Guidelines no. OPPTS 830.6316: "Explodability", August 1996.

11.2. Statement

A test item is considered explosive when it can react to produce very rapid increases in temperature or pressure.

The purity/composition of the test item is shown in Appendix 1. None of the components of the test item does contain chemical groups which are associated with explosive properties. The molecular structures of impurities at < 1% were not taken into account.

In conclusion, MLA-3202 has no explosive properties.

12. AUTO-IGNITION TEMPERATURE

12.1. Guidelines

- European Community (EC), EC no. 440/2008, Part A: Methods for the Determination of Physico-Chemical Properties, Guideline A.15: "Auto-Ignition Temperature (Liquids and Gases)", Official Journal of the European Union no. L142, May 31, 2008.
- Deutsches Institut für Normung (DIN), DIN Guide 51794: "Determining the Ignition Temperature of Petroleum Products", May 2003.
- International Electrotechnical Commission (IEC), IEC standard 79-4: "Electrical Apparatus for Explosive Gas Atmospheres, Part 4, Method of Test for Ignition Temperature", 1975.

12.2. Performance of the test

The auto-ignition temperature of the test item was determined using a commercially available auto-ignition temperature apparatus (Chilworth Technology, Southampton, UK). The method is applicable to test items with an auto-ignition temperature in the range 75°C – 650°C.

In every ignition test, liquefied test item was introduced into a preheated test vessel using a volumetric pipette. It was observed visually whether a reaction (clearly perceptible flame and/or explosion) of the sample within five minutes after introduction took place at the prevailing temperature. After each ignition test, any vaporizable components left in the flask were blown out with air (Air Products, Amsterdam, The Netherlands).

12.2.1. Preliminary test

Starting at 200°C, for every 20°C temperature rise, 70 µL test item was introduced into the test vessel until ignition of the test item was first observed (i.e. at 380°C).

Starting at 390°C, for every 5°C decrease, 70 µL test item was tested until no ignition of the test item had been observed. The temperature at which ignition was last observed is the estimated auto-ignition temperature.

12.2.2. Main study

Three tests were performed. The sample volumes applied and temperature range of each test are given below. Starting at the "high temperature", for every 2°C decrease, the prevailing volume of test item was tested until no ignition of the test item had been observed. The temperature at which ignition was last observed is the auto-ignition temperature at the sample volume applied. This procedure was repeated with the other volumes until a minimum auto-ignition temperature for each test was obtained. With these results the auto-ignition temperature of the test item was determined.

The atmospheric pressure during the performance of the main study was between 1008.2 and 1015.5 hPa.

Test	Volume [µL]	Temperature (°C)	
		start	end
Test 1	70	389	369
	150	368	364
	300	365	361
	600	374	370
Test 2	100	377	369
	250	370	368
	350	369	367
	400	367	363
	550	374	370
Test 3	125	376	364
	325	365	361
	625	379	375

12.3. Interpretation

The degree of auto-ignitability is expressed in terms of the auto-ignition temperature. The auto-ignition temperature is the lowest temperature at which the test item ignites when mixed with air under the conditions defined in the test method.

12.4. Results

12.4.1. Preliminary test

The estimated auto-ignition temperature was 380°C.

12.4.2. Main study

The results of the main study on the determination of the auto-ignition temperature of the test item are given in [Table 6](#).

Ignition of the test item within 5 minutes after introduction was observed with each sample volume and with each test a minimum auto-ignition temperature was obtained. The maximum deviation between the three values was < 20°C. According to the guidelines, no further testing was required.

The lowest temperature at which ignition of the test item occurred was 363°C. This temperature was rounded down to the nearest multiple of 5°C giving an auto-ignition temperature of the test item of 360°C.

Table 6
Main study - auto-ignition temperature of the test item

Test	Volume [µL]	Auto-ignition temperature [°C]	Ignition delay [s]	Colour of the flame	Minimum auto-ignition temperature [°C]
1	70	371	10	Orange	363
	150	366	11	Orange/Blue	
	300	363	12	Orange/Blue	
	600	372	12	Orange/Blue	
2	100	371	8	Orange	365
	250	370	8	Orange/Blue	
	350	369	7	Orange/Blue	
	400	365	10	Blue	
	550	372	12	Blue	
3	125	366	11	Orange	363
	325	363	13	Orange/Blue	
	625	377	13	Orange/Blue	

12.5. Conclusion

Commercially available auto-ignition temperature apparatus was used for the determination of the degree of auto-ignitability of MLA-3202..

The test item is auto-ignitable with an auto-ignition temperature of 360°C at 1008.2 – 1015.5 hPa.

13. OXIDIZING PROPERTIES

13.1. Guidelines

- European Community (EC), EC no. 440/2008, Part A: Methods for the Determination of Physico-Chemical Properties, Guideline A.21: "Oxidizing Properties (Liquids)", Official Journal of the European Union no. L142, May 31, 2008.
- United Nations (UN), UN no. ST/SG/AC.10/11/Rev.6: Recommendations on the Transport of Dangerous Goods, Part III: Classification Procedures, Test Methods and Criteria Relating to Class 2, Class 3, Class 4, Division 5.1, Class 8 and Class 9, Test O.2: "Test for Oxidizing Liquids", 2015.
- United Nations (UN), UN no. ST/SG/AC.10/11/Rev.6: Recommendations on the Transport of Dangerous Goods, Appendix 6: "Screening Procedures", 2015.

13.2. Statement

A test item is considered an oxidizing substance when a mixture of the substance and cellulose in a 1:1 ratio (by mass) spontaneously ignites or the mean pressure rise time of the mixture is less than or equal to mean pressure rise time of a 1:1 reference mixture (by mass) of 65% aqueous nitric acid and cellulose.

The purity of the test item is shown in appendix 1. None of the components of the test item does contain groups that act as an oxidizing agent. The oxygen atoms that are present in the molecular structure of the test item are chemically bonded to carbon or hydrogen. The molecular structures of impurities at < 1% were not taken into account.

In conclusion, MLA-3202 has no oxidizing properties.

14. DISSOCIATION CONSTANTS

14.1. Guideline

Organization for Economic Co-operation and Development (OECD), OECD Guidelines for Testing of Chemicals, Guideline no. 112: "Dissociation Constants in Water" Adopted May, 12 1981.

United States Environmental Protection Agency (EPA), Product Properties Test Guidelines no. OPPTS 830.7370: "Dissociation Constants in Water, August 1996.

14.2. Test system

14.2.1. Calculation method

Software pK_a Perrin calculation method (pKalc 5.0, module in Pallas 3.0, CompuDrug International, San Francisco, CA, USA).

14.3. Performance of the test

14.3.1. Calculation method

The pK_a values calculated for C16:0 (palmitic) tallow amides, N-N-bis(2-hydroxypropyl) and C18:2 (linoleic) tallow amides, N-N-bis(2-hydroxypropyl), ingredients in MLA-3202 were calculated from their structure using Perrin's calculation method. For this, a computer program was used. The operation of the computer program is described in the pKalc user's manual.

14.4. Interpretation

14.4.1. Calculation method

K_a is the acidic ionisation constant and pK_a is the negative logarithm of K_a.

14.5. Results

14.5.1. Calculation method

Perrin's calculation method was used to calculate the pK_a values for the acidic and basic groups in C16:0 (palmitic) tallow amides, N-N-bis(2-hydroxypropyl), ingredients in MLA-3202.

<i>Acidic groups</i>		<i>Basic groups</i>	
RRCHOH	14.71	RCON(R)2	-0.70
	15.76		

Perrin's calculation method was used to calculate the pK_a values for the acidic and basic groups in C18:2 (linoleic) tallow amides, N-N-bis(2-hydroxypropyl), ingredients in MLA-3202.

<i>Acidic groups</i>		<i>Basic groups</i>	
RRCHOH	14.71	RCON(R)2	-0.70
	15.76		

14.6. Conclusion

Since other ingredients in MLA-3202 have structures similar to that of C16:0 (palmitic) tallow amides, N-N-bis(2-hydroxypropyl) and C18:2 (linoleic) tallow amides, N-N-bis(2-hydroxypropyl), it is concluded that ingredients in MLA-3202 do not contain any groups that are ionised in the pH range 1-13.

15. APPEARANCE

15.1. Guidelines

United States Environmental Protection Agency (EPA), Product Properties Test Guidelines no. OPPTS 830.6302: "Color", August 1996.

United States Environmental Protection Agency (EPA), Product Properties Test Guidelines no. OPPTS 830.6303: "Physical State", August 1996.

United States Environmental Protection Agency (EPA), Product Properties Test Guidelines no. OPPTS 830.6304: "Odor", August 1996.

15.2. Performance

The physical state, color and, if characteristic, odour of the formulation were determined.

For determination of the appearance of the formulation, a 6.3697 g sample was taken from the test item, transferred into a 20 mL glass vial and observed against a white background. The physical state was described. The color was compared with the Munsell color-order system (The Munsell book of color, Macbeth, Division of Kollmorgen Instruments Corporation, New Windsor, New York, USA). The observations were performed in a fume cupboard at a temperature between 19.5°C and 22.5°C.

15.3. Results

15.3.1. Appearance of formulation

MLA-3202 was an amber colored, clear liquid (Munsell code 8.75 YR 7/14). No characteristic odour was noticed during handling of the test item.

16. PH, ACIDITY - ALKALINITY

16.1. Guidelines

CIPAC, Analysis of Technical and Formulated Pesticides, MT 75.3: "Determination of pH values", CIPAC Handbook Volume J, 2000.

Organization for Economic Co-operation and Development (OECD), OECD Guideline for the Testing of Chemicals no. 122: "Determination of pH, Acidity and Alkalinity", 26 July 2013.

United States Environmental Protection Agency (EPA), Product Properties Test Guidelines no. OPPTS 830.7000: "pH", August 1996.

16.2. Reagents

Double distilled water	Waldeck, Münster-Roxel, Germany
Potassium hydrogen phthalate (C ₈ H ₅ KO ₄)	Merck, Darmstadt, Germany
Di-sodium tetraborate decahydrate (Na ₂ B ₄ O ₇ .10H ₂ O)	Sigma-Aldrich, Steinheim, Germany
0.05M buffer solution pH 4.00 ± 0.02	10.21 g potassium hydrogen phthalate dried for 2 hours at 105°C, dissolved in double distilled water and made up to 1000 mL.
0.05M buffer solution pH 9.22 ± 0.02	19.07 g di-sodium tetraborate decahydrate dissolved in double distilled water and made up to 1000 mL.

All reagents were of analytical grade, unless specified otherwise.

16.3. Performance of the test

The pH of two 1% (w/v) mixtures of the test item in double distilled water was measured using a 906 Titrando (Metrohm, Herisau, Switzerland) and a combined glass electrode (glass/glass electrode and reference electrode, Metrohm). Also the pH of the undiluted test item will be measured in duplicate.

The pH meter was calibrated using a 0.05 M potassium hydrogen phthalate buffer solution (pH 4.00) and a 0.05 M di-sodium tetraborate buffer solution (pH 9.22 at 20°C).

At the start and at the end of the measurements, pH of these buffer solutions was measured to ensure proper performance of the pH meter.

For the preparation of the 1% (w/v) mixtures, accurately weighed amounts of 1.0006 g and 1.0009 g of the test item were transferred into a 100 mL measuring cylinder, containing about 50 mL water. The volume was made up to 100 mL with water, the cylinder was stoppered and the dispersion was shaken vigorously by hand until completely mixed or dispersed. After it was left to stand for 1 minute, the combined glass electrode was immersed into the liquid and the pH was measured without stirring. The pH value was recorded after 1 and 2 minutes.

Because the pH value changed more than 0.1 unit during this equilibration time, the pH was also recorded 10 minutes after immersion of the electrode.

The pH of the undiluted test item was determined directly. The electrode was immersed into the test item and the pH value was recorded after 1 and 2 minutes.

The test was performed at $23.2 \pm 0.8^\circ\text{C}$.

16.4. Interpretation

The pH value of an aqueous liquid is defined as the logarithm to the base ten of the reciprocal of the hydrogen ion concentration expressed in mol/L.

16.5. Results

The results of the test on the determination of the pH of the test item are given in [Table 7](#).

The 1% (w/v) mixtures of the test item in double distilled water were opaque white suspensions with approximately 5 mL white foam.

Table 7 pH of the test item

	Test item	pH 1% (w/v) mixture
	6.495 6.561	4.693 4.671
mean	6.5	4.7

16.6. Conclusion

The pH of the undiluted test item and of 1% (w/v) aqueous mixtures of the test item was measured using a 906 Titrando (Metrohm, Herisau, Switzerland).

The pH of the test item was 6.5.

The pH of the 1% (w/v) aqueous mixtures was 4.7.

17. VISCOSITY

17.1. Guidelines

- Organization for Economic Co-operation and Development (OECD), OECD Guidelines for the Testing of Chemicals no. 114: "Viscosity of Liquids", October 2, 2012.
- United States Environmental Protection Agency (EPA), Product Properties Test Guidelines no. OPPTS 830.7100: "Viscosity", August 1996.
- International Organization for Standardization (ISO), ISO 3104: "Petroleum Products - Transparent and Opaque Liquids - Determination of Kinematic Viscosity and Calculation of Dynamic Viscosity", 1994.
- ASTM International, ASTM D 445-09: "Standard Test Method for Kinematic Viscosity of Transparent and Opaque Liquids (and Calculation of Dynamic Viscosity)", July 1, 2009.

17.2. Performance of the test

The viscosity of the test item was determined at 20°C and 40°C using a glass capillary viscometer (Tamson Instruments, Bleiswijk, The Netherlands).

Based on information supplied by the sponsor, the Ubbelohde viscometers with constants 0.4685 and 0.9067 mm²/s² were selected. The viscometer was charged with the test item by tilting it about 30° from the vertical position. When the viscometer was returned to the vertical the meniscus of the test item was between the filling marks of the reservoir bulb.

The viscometer was placed in the thermostatic water bath and remained in the bath for at least 30 minutes to reach the test temperature.

The test item was drawn by vacuum through the timing tube to about 5 mm above the upper timing mark. The vacuum was released. The time required for the meniscus to pass from the upper to the lower timing mark was measured and the kinematic viscosity of the test item was determined.

The kinematic viscosity of the test item was determined at 20 ± 0.1°C and 40 ± 0.1°C. Each test was performed in duplicate.

17.3. Interpretation

17.3.1. Specifications

The kinematic viscosity is defined as the resistance to flow of a fluid under gravity. The kinematic viscosity is expressed in mm²/s.

17.3.2. Formulas

Kinematic viscosity

$$\nu = C \times t$$

where:

C = calibration constant [mm²/s²]

t = flow time [s]

17.4. Results

The results for the kinematic viscosity of the test item at 20°C and 40°C are given in [Table 8](#).

Table 8
Viscosity of the test item

Temperature [°C]	Test	Calibration constant [mm ² /s ²]	Flow time [s]	Kinematic viscosity [mm ² /s]	Mean [mm ² /s]
20	I	0.4685	2380	1115	1116
	II	0.9067	1231	1116	
40	I	0.4685	520	244	245
	II	0.9067	271	245	

17.5. Conclusion

The viscosity of MLA-3202 was determined using a glass capillary viscometer.

The kinematic viscosity of the test item was:

	Kinematic viscosity [mm ² /s]	
	20°C	40°C
Test item	1116	245

18. FLAMMABILITY IN CONTACT WITH WATER

18.1. Guidelines

- European Community (EC), EC no. 440/2008, Part A: Methods for the Determination of Physico-Chemical Properties, Guideline A.12: "Flammability (Contact with Water)", Official Journal of the European Union no. L142, May 31, 2008.
- United Nations (UN), UN no. ST/SG/AC.10/11/Rev.6: Recommendations on the Transport of Dangerous Goods, Part III: Classification Procedures, Test Methods and Criteria Relating to Class 2, Class 3, Class 4, Division 5.1, Class 8 and Class 9, Test N.5: "Test Method for Substances which in Contact with Water Emit Flammable Gases", 2015.
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18.2. Statement

A test item is considered highly flammable when it ignites spontaneously in contact with water, or evolves a flammable gas at a minimum rate of ≥ 1 litre/kg of the substance per hour.

The purity/composition of the test item is shown in Appendix 1. None of the components of the test item does contain groups that might lead to ignition in contact with water and/or to the evolution of a flammable gas. Moreover the test item was dissolved in water during the determination of the surface tension (see chapter 9). It demonstrated that the test item does not ignite spontaneously in contact with water. The molecular structures of impurities at < 1% were not taken into account.

In conclusion, MLA-3202 is considered 'not highly flammable' in contact with water.

Appendix 1

Certificate of analysis



Chempura Corporation
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Naugatuck, CT 06770

Analytical Services
www.chemtura.com

Certificate of Purity

Customer: Support for Toxicology Studies

Test Substance Name: MLA3202; Amides, tallow, N,N-bis(2-hydroxypropyl)

Physical Appearance: Liquid

CAS No.: 1454803-04-3

Ref. or Lot Number: RC-1045

Date of Analysis: revised March 18, 2016 (original issue March 7, 2016)

Percent Composition	Monoisotopic Mass (daltons)	Formula	Structure/ Identity
33.1	397.4	C ₂₄ H ₄₇ NO ₃	C18:1 (oleic) tallow amides, N,N-bis(2-hydroxypropyl)
22.9	371.3	C ₂₂ H ₄₅ NO ₃	C16:0 (palmitic) tallow amides, N,N-bis(2-hydroxypropyl)
13.6	395.4	C ₂₄ H ₄₅ NO ₃	C18:2 (linoleic) tallow amides, N,N-bis(2-hydroxypropyl)
11.0	399.4	C ₂₄ H ₄₉ NO ₃	C18:0 (stearic) tallow amides, N,N-bis(2-hydroxypropyl)
6.0	369.3	C ₂₂ H ₄₃ NO ₃	C16:1 (palmitoleic) tallow amides, N,N-bis(2-hydroxypropyl)
3.2	419.3	C ₂₆ H ₄₅ NO ₃	C20:4 (eicosatetraenoic) tallow amides, N,N-bis (2-hydroxypropyl)
2.0	393.3	C ₂₄ H ₄₃ NO ₃	C18:3 (linolenic) tallow amides, N,N-bis(2-hydroxypropyl)
1.5	282.3	C ₁₈ H ₃₄ O ₂	C18:1 (oleic) acid
1.1	421.4	C ₂₆ H ₄₇ NO ₃	C20:3 (eicosatrienoic) tallow amides, N,N-bis (2-hydroxypropyl)
5.6			Sum of residual components (< 1% each)
100.0			Total

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